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SUBJECT: **PHYSICALLY MOTIVATED FALSE CONVERGENCE PROTECTION**

The zero-variance biasing derived in [1] was implemented in a test code and the convergence rate was better than the square root of the number of samples in some cases. In other cases, false convergence to the wrong mean was observed. After examining the false convergence displayed, I was able to see what was going wrong as a violation of some physical constraints. This memo derives these constraints.

Note that the general idea behind the constraints derived herein is similar to Henry Lichtenstein's work[2]. Both methods use *known* local information about the underlying transport process to compare against the learned simulation results.

Consider a bidirectional transport problem along the x-axis. The particles can move only forward or backward on the interval  $(0, T)$ . A unit weight particle source is started moving forward at  $x = 0$ . The desired estimate is the number of particles escaping at  $x = T$ .

Definition 1.

$$L(x) = \text{expected score of a unit weight particle at } x \text{ moving backward} \quad (1)$$

Definition 2.

$$N(x) = \text{expected score of a unit weight particle at } x \text{ moving forward} \quad (2)$$

Definition 3.

$$\sigma = \text{total macroscopic cross section} \quad (3)$$

Definition 4.

$$\sigma_s = \text{total scattering cross section} \quad (4)$$

Definition 5.

$$f = \text{probability of no direction change upon scatter} \quad (5)$$

Definition 6.

$$b = \text{probability of direction reversal upon scatter} \quad (6)$$

In the test code,  $N(x)$  and  $L(x)$  are unknown and must be estimated. The estimates of  $N(x)$  and  $L(x)$  are then used for biasing the next Monte Carlo transport calculation in an iterative fashion.

The physical constraints on  $N(x)$  and  $L(x)$  started from Eqs. 28 and 46 of [1]. These equations are now repeated. For a particle at  $x$  moving forward, the weight multiplication upon collision at  $x + s$  is

$$w_c(x + s) = \frac{\sigma N(x)}{\sigma N(x + s) - N'(x + s)} \quad (7)$$

(The prime indicates the derivative). For a particle at  $x$  moving backward, the weight multiplication upon collision at  $x - s$  is

$$w_c(x - s) = \frac{\sigma L(x)}{\sigma L(x - s) + L'(x - s)} \quad (8)$$

The most obvious physical constraints are that the expected score must be nonnegative,

$$N(x) \geq 0 \quad (9)$$

$$L(x) \geq 0 \quad (10)$$

and the denominators of Eqs. 7 and 8 must be positive

$$\sigma N(x + s) - N'(x + s) > 0 \quad (11)$$

$$\sigma L(x - s) + L'(x - s) > 0 \quad (12)$$

Just imposing constraints 9-12 alleviated the false convergence problem in most cases. However, there were occasional problems when Eqs. 11 or 12 were just barely satisfied. This meant very large weight multiplications at some collisions. False convergence tended to occur when none of these large weight multiplications occurred and nonconvergence tended to occur when they occurred. By nonconvergence it is meant that the iterative learning process failed and the calculational efficiency did not improve with each iteration. A way was needed to bound Eqs. 11 and 12 away from zero.

First, consider a particle moving in the forward direction at  $x$ . The set of next events (for an analog particle) may be partitioned into four possibilities:

1. With probability  $1 - \sigma dx$  the particle does not collide in  $dx$  and its expected score at  $x + dx$  is then  $N(x + dx)$ .
2. The particle collides in  $dx$  with probability  $\sigma dx$  and then is absorbed with probability  $(1 - \sigma_s/\sigma)$ . Thus, an absorption occurs in  $dx$  with probability  $\sigma dx(1 - \sigma_s/\sigma)$ . The expected score after absorption is zero.
3. The particle collides in  $dx$  with probability  $\sigma dx$ , survives the collision with probability  $\sigma_s/\sigma$ , and then scatters forward with probability  $f$ . Thus with probability  $\sigma dx(\sigma_s/\sigma)f$  the particle will have an expected score between  $N(x)$  and  $N(x + dx)$ . Because the probability already has a  $dx$  term, then to first order we may take the expected score as  $N(x)$ .
4. The particle collides in  $dx$  with probability  $\sigma dx$ , survives the collision with probability  $\sigma_s/\sigma$ , and then scatters backward with probability  $b$ . Thus with probability  $\sigma dx(\sigma_s/\sigma)b$  the particle will have an expected score between  $L(x)$  and  $L(x + dx)$ . Because the probability already has a  $dx$  term, then to first order we may take the expected score as  $L(x)$ .

Using the above partition, the expected score at  $x$  may be written as

$$N(x) = (1 - \sigma dx)N(x + dx) + \sigma dx[1 - (\sigma_s/\sigma)] \cdot 0 + \sigma dx(\sigma_s/\sigma)fN(x) + \sigma dx(\sigma_s/\sigma)bL(x) \quad (13)$$

Rearranging Eq. 13,

$$[-f\sigma_s N(x) + \sigma N(x + dx)]dx = N(x + dx) - N(x) + \sigma_s dx b L(x) \quad (14)$$

Now dividing Eq. 14 by  $dx$  and letting  $dx \rightarrow 0$  yields

$$N(x)(\sigma - \sigma_s f) = N'(x) + \sigma_s b L(x) \quad (15)$$

Because the last term on the right hand side is nonnegative,

$$N(x)(\sigma - \sigma_s f) - N'(x) \geq 0 \quad (16)$$

If this is required everywhere, then the denominator in Eq. 7 is bounded away from zero, except when  $N(x) = L(x) = 0$ .

Second, consider a particle moving in the backward direction at  $x$ . The set of next events (for an analog particle) may be partitioned into four possibilities:

1. With probability  $1 - \sigma dx$  the particle does not collide in  $dx$  and its expected score at  $x - dx$  is then  $L(x - dx)$ .

2. The particle collides in  $dx$  with probability  $\sigma dx$  and then is absorbed with probability  $(1-\sigma_s/\sigma)$ . Thus, an absorption occurs in  $dx$  with probability  $\sigma dx(1-\sigma_s/\sigma)$ . The expected score after absorption is zero.
3. The particle collides in  $dx$  with probability  $\sigma dx$ , survives the collision with probability  $\sigma_s/\sigma$ , and then forward scatters with probability  $f$ . Thus with probability  $\sigma dx(\sigma_s/\sigma)f$  the particle will have an expected score between  $L(x)$  and  $L(x-dx)$ . Because the probability already has a  $dx$  term, then to first order we may take the expected score as  $L(x)$ .
4. The particle collides in  $dx$  with probability  $\sigma dx$ , survives the collision with probability  $\sigma_s/\sigma$ , and then backward scatters with probability  $b$ . Thus with probability  $\sigma dx\sigma_s/\sigma b$  the particle will have an expected score between  $N(x)$  and  $N(x-dx)$ . Because the probability already has a  $dx$  term, then to first order we may take the expected score as  $N(x)$ .

Using the above partition, the expected score at  $x$  may be written as

$$L(x) = (1 - \sigma dx)L(x - dx) + \sigma dx[1 - (\sigma_s/\sigma)] \cdot 0 + \sigma dx(\sigma_s/\sigma)fL(x) + \sigma dx(\sigma_s/\sigma)bN(x) \quad (17)$$

Rearranging Eq. 17,

$$[-f\sigma_s L(x) + \sigma L(x - dx)]dx = L(x - dx) - L(x) + \sigma_s dx b N(x) \quad (18)$$

Now dividing Eq. 18 by  $dx$  and letting  $dx \rightarrow 0$  yields

$$L(x)(\sigma - \sigma_s f) = -L'(x) + \sigma_s b N(x) \quad (19)$$

Because the last term on the right hand side is nonnegative,

$$L(x)(\sigma - \sigma_s f) + L'(x) \geq 0 \quad (20)$$

If this is required everywhere, then the denominator in Eq. 8 is bounded away from zero, except when  $N(x) = L(x) = 0$ .

Note that Eqs. are special cases of Eqs. 47 and 48 in [3]. However, it was easier to derive the equations here than to treat them as special cases of Eqs. 47 and 48.

## REFERENCES

- [1] **Zero Variance Biasing Derivation**, LANL memorandum XTM:96-184 (U), Thomas E. Booth May 6, 1996

- [2] **Studies in False Learning – III**, LANL memorandum XTM:96-115 (U), Henry Lichtenstein March 13, 1996
- [3] **Analytic Score Distributions and Moments for a Spatially Continuous Tridirectional Monte Carlo Transport Problem**, LA-12570 July 1993, Thomas E. Booth

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